Block Reflectors: Theory and Computation

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BLOCK REFLECTORS: THEORY AND COMPUTATION*

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Abstract. A block reflector is an orthogonal, symmetric matrix that reverses a subspace whose dimension may be greater than one. We shall develop the properties of block reflectors and give some algorithms for computing a block reflector that introduces a block of zeros into a matrix. We consider the compact representation of block reflectors, some applications, and their use in parallel computers.

1. Introduction.

Block reflectors are orthogonal, symmetric matrices with possibly more than one negative eigenvalue. They are a natural generalization of the elementary reflectors (also known as Householder transformations) that are widely used in matrix computation. Block reflectors have similar uses.

We shall develop a theory of block reflectors and their computation. We also discuss some applications of block reflectors, give some numerical results showing the stability of our algorithm, and show how this algorithm is well matched to the capabilities of some new, fast scientific computers.

Block reflectors are not new. Brønlund and Johnsen gave a method for orthogonal reduction to block upper triangular form, but the orthogonal transformations were nonsymmetric [2]. Dietrich derived the block reflector as we discuss it here, gave a stable method for computing it, and showed how it may be used for reduction to block upper triangular form [4]. Kaufman has considered the use of block reflectors for block triangularization of a sparse matrix [8].

In this paper, we make the following contributions. First, we derive a complete theory of block reflectors, clearly showing the parallels between the block and the point theory. Our presentation is considerably more direct than that found in [4].

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In addition to existence, we also answer the question of the uniqüeness of the block reflector, giving it in its most general form. Then we present a new view of the theory; our vantage point is the operator angle between two subspaces. This more clearly reveals the structure of the block reflector used to map between two subspaces, and also leads to new algorithms.

After providing two applications, we show how to construct a block reflector that introduces a zero block into a matrix. Four algorithms are presented. One is a new version of Dietrich's stable method. The role played by the polar decomposition of a matrix in this method is revealed. A second, related algorithm can be used to construct any of the several block reflectors that map between a given pair of subspaces; Dietrich's method can be used to construct only one of these. Two new algorithms based on the operator angle are also given. Finally, the efficiency of these methods on modern parallel computers is examined. A numerical experiment illustrates their accuracy, even for very badly conditioned matrices.

Bischof and Van Loan have pursued a somewhat different approach [1]. They develop a representation for the product of several elementary reflectors of the form $I - WY$, where W and Y are rectangular matrices. With this representation, the usual orthogonal reduction to triangular form can be organized so that it is dominated by matrix multiplications, an important virtue, as we explain below.

For any matrix X, $R(X)$ denotes the range of X. For any subspace Y, $Y^{\perp}$ denotes the orthogonal complement of Y.

2. Block reflectors: Theory.

2.1. Definition. Given any $Z \in \mathbf{R}^{m\times n}$, $m \geq n$, "the reflector that reverses the range of Z" is given by

$$H = H(Z) := I_m - ZWZ^t$$

where

$$W = 2(Z^tZ)^+ \in \mathbf{R}^{n\times n}$$

is the (symmetric) pseudo-inverse of $\frac{1}{2}(Z^tZ)$. (See [6, p. 139] for a fuller description of the pseudo-inverse.) Thus

$$ZWZ^t = 2P_Z$$

where P_Z is the orthogonal projector on $R(Z)$.

When $n = 1$, H is an elementary reflector or Householder transformation. When Z^tZ is invertible, $W = (\frac{1}{2}Z^tZ)^{-1}$. Note that if $Z = 0$, then $W = 0$ and $H(0) = I$. Also, $H(Z)Z = -Z$. (See Lemma 1 for proof.)

This choice of W makes H orthogonal as well as symmetric. Hence, $H^2 = I$, the reflector property.

It is also easy to verify that if $R(Z) = R(Z_1)$, then $H(Z) = H(Z_1)$. Thus, for example, $H(ZT) = H(Z)$ for any invertible T, and $H(ZW) = H(Z)$ as well.

Since H is orthogonal and symmetric, its eigenvalues are 1 and -1. The multiplicity of -1 is equal to the dimension of the space reversed by H; this in turn is equal to the rank of Z.

2.2. Essential properties. Every $m \times m$ orthogonal reflector H induces a decomposition of $\mathbf{R}^m$ into the direct sum of two perpendicular subspaces; one subspace is H invariant and the other is reversed by H. The following lemma states that for the reflector $H(Z)$, the reversed subspace is $R(Z)$.

LEMMA 1. *Let $Z \in \mathbf{R}^{m\times n}$. For all $z \in R(Z)$,*

$$H(Z)z = -z \tag{1a}$$

and for all $y \in R(Z)^{\perp}$,

$$H(Z)y = y\,. \tag{1b}$$

Proof. We require the fact that, for any matrix B,

$$B(B^tB)^+B^tB = B\,,$$

which is easy to prove using the singular value decomposition (SVD) of B. (See [6, pp. 16-20] for more information on the SVD.) Now let $z \in R(Z)$. Then there exists x, such that $z = Zx$. Using the fact above and the definition of $H(Z)$,

$$\begin{aligned} H(Z)z &= Zx - ZWZ^tZx \\ &= Zx - 2Zx \\ &= -z \end{aligned}$$

so that (1a) is proved. Property (1b) comes from applying $H(Z)$ to y and noting that $Z^ty = 0$. QED

2.3. The standard task. Let $E = \begin{pmatrix} E_1 \\ E_2 \end{pmatrix} \in \mathbf{R}^{m\times n}$, with $m > n$, and E_1 square. We seek a block reflector H such that

$$HE = \overline{F} := \begin{pmatrix} F \\ 0 \end{pmatrix}$$

with F square. We now give conditions on F that are necessary and sufficient for the existence of H:

(2a) ISOMETRY PROPERTY: $F^tF = E^tH^tHE = E^tE$

and

(2b) SYMMETRY PROPERTY: $E_1^tF = E^tHE = \text{symmetric}.$

Define the associated matrices:

$$D := \overline{F} - E = \begin{bmatrix} F - E_1 \\ -E_2 \end{bmatrix} \tag{3a}$$

and

$$S := \overline{F} + E. \tag{3b}$$

(D is for "difference," S is for "sum.")

An important consequence of the conditions (2) is this:

LEMMA 2. *If F satisfies* (2), *then*

$$D^t S = 0.$$

Proof. By (2),

$$\begin{aligned} D^t S &= (\overline{F}^t \overline{F} - E^t E) + (\overline{F}^t E - E^t \overline{F}) \\ &= (F^t F - E^t E) + (F^t E_1 - E_1^t F) \\ &= 0 + 0 . \end{aligned}$$

QED

THEOREM 1. *There exists a block reflector H such that $HE = \overline{F}$ if and only if F satisfies* (2).

Proof. Necessity is clear: equation (2a) follows from the orthogonality of H, while (2b) is obvious from the symmetry of H.

To show sufficiency we shall prove that $H(D)E = \overline{F}$. Since $E = \frac{1}{2}(S - D)$, we have

$$\begin{aligned} H(D)E &= \frac{1}{2}[H(D)S - H(D)D] , \\ &= \frac{1}{2}[S + D] \qquad \text{(using Lemmas 1 and 2)} \\ &= \overline{F}. \end{aligned}$$

QED

Clearly if F satisfies (2) then $-F$ does too. Furthermore, $H(S)E = -\overline{F}$. If F and E satisfy (2) we shall say that F is a *mirror image* of E.

The concept of a block reflector, the necessary and sufficient conditions, and a solution to the standard task for the case $n = 2$ were given by Tang Ling in an unpublished manuscript [10].

2.3.1. Representing H. It may not be advisable to represent H by E, F, and W as above. This form is very attractive if E must be preserved or when E is sparse. On the other hand, when E has rank $r < n$, then it saves storage to find an $m \times r$ matrix G such that $H = I - GG^t$, and $G^tG = 2I_r$. (We later show that this is possible). Storage of G requires mr words, as opposed to $mn + n^2$ for Z and W, $mn + 2n^2$ for E, F, and W, and $2mn$ for the WY representation of Bischof and Van Loan. Computing Hx for a vector x costs $2mr$ flops (1 flop is one multiply and one add) compared with $2mn + n^2$ for the Z, W representation. An algorithm for computing G is given in §3.2.

2.4. The form of F. F is far from unique, even when E has full rank n. If $E_1 = 0$ then the symmetry condition is vacuous and we may choose any F satisfying the isometry condition $F^tF = E^tE$. At the other extreme, when E_1 is invertible, then F must have the form $F = ME_1$ with M symmetric. Now the isometry condition requires

$$M^2 = E_1^{-t}(E^tE)E_1^{-1} .$$

There are 2^n solutions, namely $M = V \operatorname{diag}(\pm\sqrt{\lambda_1}, \pm\sqrt{\lambda_2}, \cdots, \pm\sqrt{\lambda_n})V^t$ where

$$E_1^{-t}(E^tE)E_1^{-1} = V \operatorname{diag}(\lambda_1, \cdots, \lambda_n)V^t$$

is the spectral factorization. Note that there are 2^n different solutions for every spectral factorization of $E^{-t}(E^tE)E^{-1}$. And with repeated eigenvalues there are infinitely many such factorizations.

The two "extreme" solutions are $F = \pm\left[E_1^{-t}(E^tE)E_1^{-1}\right]^{1/2} E_1$, where $A^{1/2}$ is the positive definite square root of A.

Example. Let

$$E = \begin{bmatrix} V \\ 0 \end{bmatrix}$$

where $V^t = V^{-1}$; i.e., V is orthogonal. Then $E_1^{-t}(E^tE)E_1^{-1} = VV^t = I$. Thus we may take M to be *any* symmetric orthogonal matrix ($M^2 = I$); in particular, $M = I$ will do. Then $F = MV$, and

$$HE = \begin{pmatrix} M & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} V \\ 0 \end{pmatrix} = \begin{pmatrix} F \\ 0 \end{pmatrix} .$$

2.4.1. The general case. Let $E_1 = P\Sigma Q^t$ with $P^tP = Q^tQ = I_{r_1}$, Σ positive definite and diagonal, $r_1 \le n$. This is the "short" SVD of E_1, where $r_1 = \operatorname{rank}(E_1)$. The symmetry condition (2b) requires that

$$Q\Sigma P^t F = \text{symmetric} .$$

The general solution for F is

$$F = (P, \tilde{P}) \begin{pmatrix} M_{11} & 0 \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} \Sigma & 0 \\ 0 & I_{n-r_1} \end{pmatrix} (Q, \tilde{Q})^t ,$$

where $\tilde{P}$, $\tilde{Q} \in \mathbf{R}^{n\times(n-r_1)}$ make $(P, \tilde{P})$ and $(Q, \tilde{Q})$ orthogonal. M_{11} must be symmetric, but M_{21} and M_{22} are free.

The isometry condition (2a) yields

$$\begin{pmatrix} M_{11} & M_{21}^t \\ 0 & M_{22}^t \end{pmatrix} \begin{pmatrix} M_{11} & 0 \\ M_{21} & M_{22} \end{pmatrix} = \begin{pmatrix} \Sigma^{-1} & 0 \\ 0 & I \end{pmatrix} (Q, \tilde{Q})^t E^t E (Q, \tilde{Q}) \begin{pmatrix} \Sigma^{-1} & 0 \\ 0 & I \end{pmatrix}$$

For each choice of $\tilde{P}$ and $\tilde{Q}$ we can find M_{11}, M_{21}, and M_{22} such that this equation holds. The solutions are not unique. We solve

$$\text{(4a)} \qquad M_{22}^t M_{22} = \tilde{Q}^t E^t E \tilde{Q},$$

$$\text{(4b)} \qquad M_{22}^t M_{21} = \tilde{Q}^t E^t E Q \Sigma^{-1},$$

$$\text{(4c)} \qquad M_{11}^2 = \Sigma^{-1}(EQ)^t(EQ)\Sigma^{-1} - M_{21}^t M_{21}.$$

Even when M_{22} is singular, (4b) is consistent. Nevertheless, the system (4b) may be ill conditioned, so we do not propose to use (4) in computations.

2.5. Is H unique?

Suppose F satisfies the isometry and symmetry conditions (2). We have shown that the choice $Z = D$ provides a block reflector H such that $HE = \overline{F}$. Is this the only such $H(Z)$? The answer depends on the rank of D and the rank of S in (3) above.

THEOREM 2. *Let F satisfy* (2). *Let $H = H(Z)$. The conditions*

$$\text{(5a)} \qquad R(D) \subseteq R(Z)$$

and

$$\text{(5b)} \qquad R(Z) \perp R(S), \quad \text{i.e.,} \quad Z^t S = 0$$

are necessary and sufficient for $H(Z)E$ to be equal to $\overline{F}$.

Proof. Recall that $E = \frac{1}{2}(S - D)$. If Z satisfies (5) then, as in the proof of Theorem 1,

$$\begin{aligned} H(Z)E &= \frac{1}{2}(HS - HD) \\ &= \frac{1}{2}(S + D) \\ &= \overline{F} \end{aligned}$$

by Lemmas 1 and 2.

On the other hand, if $HE = \overline{F}$, then

$$\overline{F} = E - ZWZ^t E,$$

so that

$$\begin{aligned} D &= -ZWZ^tE \\ &= Z(-WZ^tE) \end{aligned}$$

which implies (5a). Now that (5a) is established. we may use it to prove that (5b) holds. A consequence of (5a) is that $H(Z)D = -D$. Rewriting this relation yields

$$ZWZ^tD = 2D\ .$$

.Using this equation we obtain

$$\begin{aligned} \overline{F} &= HE \\ &= E - \frac{1}{2}ZWZ^t(S - D) \\ &= E + D - \frac{1}{2}ZWZ^tS \\ &= \overline{F} - \frac{1}{2}ZWZ^tS\ . \end{aligned}$$

So $ZWZ^tS = 0$. Since, as we noted earlier, $\frac{1}{2}ZWZ^t$ is the orthogonal projector on $R(Z)$, the columns of S are orthogonal to those of Z . This implies (5b). QED

Now suppose that $H(Z)E = \overline{F}$. By Theorem 1, F satisfies (2) and by Theorem 2, Z satisfies (5). Let us define

$$\rho_Z = \mathrm{rank}(Z)\ , \quad \rho_D = \mathrm{rank}(D)\ , \quad \rho_S = \mathrm{rank}(S)\ .$$

Since Z, D, and S belong to $\mathbf{R}^{m \times n}$,

(6a) $$\rho_Z \leq n; \quad \rho_D \leq n; \quad \rho_S \leq n.$$

Further, by (5a)

(6b) $$\rho_D \leq \rho_Z$$

and by (5b)

(6c) $$\rho_Z \leq m - \rho_S.$$

Since F satisfies (2), Lemma 2 applies, so that

(6d) $$\rho_D + \rho_S \leq m.$$

(We could conclude (6d) from (6b) and (6c), but it is true independent of the existence of Z, as we have shown.)

Now we can say when H is unique.

THEOREM 3. *Let F be a mirror image of E. Then*

1. *if $\rho_D = n$, then $H(D)$ is the unique block reflector satisfying $HE = \overline{F}$;*
2. *if $\rho_D + \rho_S = m$, then $H(D)$ is the unique block reflector satisfying $HE = \overline{F}$;*
3. *if $\rho_D < \min(n, m - \rho_S)$, then H is not unique.*

Proof. Suppose $H(Z)E = \overline{F}$. If $\rho_D = n$, then it is clear from (5a) and (6a) that $R(Z) = R(D)$, so $H(Z) = H(D)$ is the unique block reflector that reverses $R(D)$. Similarly, if $\rho_D + \rho_S = m$, then by (5a), (5b), (6b) and (6c), we must have $R(Z) = R(D)$, and again $H(Z) = H(D)$ is the unique block reflector that reverses $R(D)$. Finally, if $\rho_D < \min(n, m - \rho_S)$, we may choose any matrix $Z \subseteq \mathbf{R}^{m \times n}$ whose range contains $R(D)$ and is orthogonal to $R(S)$. By our assumption, there exist such Z of rank $\rho_D, \rho_D + 1, \ldots, \min(n, m - \rho_S)$. QED

COROLLARY. *If E_2 has rank n, then H is unique.*

Proof. Since

$$D = \begin{pmatrix} F - E_1 \\ -E_2 \end{pmatrix},$$

it follows that $n \geq \operatorname{rank}(D) \geq \operatorname{rank}(E_2) = n$. QED

In the case of Householder transformations ($n = 1$), the condition of the corollary is satisfied unless $E_2 = 0$, in which case the standard task is not much of a task at all! Thus, like the symmetry condition (2b), the possibility of genuine nonuniqueness of the reflector H only appears in the multidimensional case.

Examples. Let

$$E = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

The three matrices

$$F_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad F_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad F_2 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

all satisfy the conditions (2). With F_0, $\rho_D = 0$ and $\rho_S = 2$ and we have $0 \leq \rho_Z \leq 1$. We may choose

$$H_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \pm 1 \end{bmatrix}.$$

With F_1 we have $\rho_D = 1$ and $\rho_S = 1$ and $1 \leq \rho_Z \leq 2$. We may choose

$$H_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & \pm 1 \end{bmatrix}.$$

With F_2 we have $\rho_D = 2$ and $\rho_S = 0$ and $2 \leq \rho_Z \leq 2$. We must choose

$$H_2 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

This example shows that nonuniqueness of F is possible and that uniqueness of H is possible even with singular E_2.

For a contrasting example, let

$$E = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}, \qquad \overline{F} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Then $\rho_D = 2$, $\rho_S = 2$. and $2 \le \rho_Z \le 2$. Thus $H = H(D)$ is unique, even though E is rank-deficient.

2.6. The angle between $R(E)$ and $R\left(\begin{bmatrix} I \\ 0 \end{bmatrix}\right)$. In this section we shall rederive many of our results using the operator angle between $R(E)$ and $R\left(\begin{bmatrix} I \\ 0 \end{bmatrix}\right)$. For a complete discussion of the angle between subspaces see Davis and Kahan [3]. This rederivation gives us a new view of the block reflector that allows some geometric insight not available otherwise. It also leads to some algorithms that would not be discovered from the algebraic perspective of the earlier sections.

Let $r \equiv \text{rank}(E)$. Let the columns of $P \in \mathbf{R}^{m \times r}$ be an orthonormal basis for $R(E)$. We discuss the problem of finding a block reflector H that performs the standard task for P rather than E; since they have the same range, this H also performs the standard task for E: If $E = PT$ and H is a block reflector such that $HP = \begin{bmatrix} Q \\ 0 \end{bmatrix}$, Q square, then $HE = \begin{bmatrix} QT \\ 0 \end{bmatrix}$. Thus, for the moment, we work with P rather than E.

Let

$$P = \begin{bmatrix} P_1 \\ P_2 \end{bmatrix}$$

where P_1 is square. Let

$$P_1 = Q_1 M_1$$

be a polar decomposition of P_1. The factor M_1 is the symmetric, nonnegative definite square root of $P_1^t P_1$, and is unique. The other factor, Q_1, is orthogonal and is unique only if P_1 is nonsingular. Since P has orthonormal columns, the eigenvalues of M_1 all lie in $[0,1]$ (see [6, p. 22]). Higham [7] discusses the polar decomposition and gives an efficient algorithm for computing it.

It is simple to show that Q_1 is a mirror image of P. In fact, a version of the converse is also true. If Q is any mirror image of P then

$$P_1 = QM$$

is a factorization of P_1 into an orthogonal-symmetric product. (The choice is in the signs of the eigenvalues of M, as it was in §2.4). For the moment we choose to work with the polar factorization.

Define $\overline{Q_1} \equiv \begin{pmatrix} Q_1 \\ 0 \end{pmatrix}$. We now write

$$M_1 = \cos 2\Theta \ ;$$

where the angle Θ is defined by

$$\Theta \equiv V \operatorname{diag}(\theta_1, \cdots, \theta_r) V^t \ ,$$

where

$$0 \le \theta_1 \le \cdots \le \theta_r \le \frac{\pi}{4} \ .$$

The eigenvectors of M_1 are the columns of V and its eigenvalues are $1 \ge \cos 2\theta_1 \ge \cdots \ge \cos 2\theta_r \ge 0$.

We also factor

(7)
$$P_2 = Q_2 M_2$$

where $M_2 = (I - M_1^2)^{1/2} = \sin 2\Theta$ is symmetric, nonnegative definite and $Q_2 \in \mathbf{R}^{m-r \times r}$. The form of Q_2 will be clarified below. We may choose Q_2 so that

(8)
$$Q_2^t Q_2 (\sin \Theta) = \sin \Theta \ .$$

It is easy to prove this by using the C-S decomposition of P [13].

From this new viewpoint we obtain several new formulas. First

$$P_1 = Q_1 M_1 = Q_1 \cos 2\Theta \ , \qquad P_2 = Q_2 M_2 = Q_2 \sin 2\Theta \ ;$$

hence

(9)
$$(I + M_1)^{1/2} = \sqrt{2} \cos \Theta \ , \qquad (I - M_1)^{1/2} = \sqrt{2} \sin \Theta \ .$$

Next,

(10)
$$S = \begin{pmatrix} Q_1 + P_1 \\ P_2 \end{pmatrix} = \begin{pmatrix} 2Q_1 \cos^2 \Theta \\ P_2 \end{pmatrix} = 2 \begin{pmatrix} Q_1 \cos \Theta \\ Q_2 \sin \Theta \end{pmatrix} \cos \Theta$$

and

(11)
$$D = \begin{pmatrix} Q_1 - P_1 \\ -P_2 \end{pmatrix} = \begin{pmatrix} 2Q_1 \sin^2 \Theta \\ -P_2 \end{pmatrix} = 2 \begin{pmatrix} Q_1 \sin \Theta \\ -Q_2 \cos \Theta \end{pmatrix} \sin \Theta \ .$$

Thus,

(12)
$$\frac{1}{2} S^t S = 2 \cos^2 \Theta$$

and

$$\frac{1}{2}D^t D = 2\sin^2\Theta \ . \tag{13}$$

The definition of the angles $\{\theta_j\}$ insures that $\cos^2\Theta$ is both nonsingular and well conditioned. Define

$$H_+ = I - G_+ G_+^t \tag{14}$$

where

$$G_+ \equiv \sqrt{2}\begin{pmatrix} Q_1\cos\Theta \\ Q_2\sin\Theta \end{pmatrix} . \tag{15}$$

By (10) and (12), since $(\cos^2\Theta)^+ = (\cos^2\Theta)^{-1}$,

$$H(S) = H_+ \ .$$

Note the analogy with the case $n = 1$ where, if 2θ is the angle between e (that is, E) and the e_1-axis, then $H = I - 2v_+v_+^t$, where $v_+ = (\cos\theta, \sin\theta)^t$.

We now consider $H(D)$. It is important to be able to construct $H(D)$ since in some instances it is what we want. In particular, if $E \approx \begin{pmatrix}\text{orthogonal}\\ 0\end{pmatrix}$ then $H(D)$ produces a small change to E.

Now note that D is not necessarily of full rank. In fact

$$\begin{aligned} \rho_D &\equiv \mathrm{rank}(D) \\ &= \mathrm{rank}(D^t D) \\ &= \mathrm{rank}(\sin\Theta) \\ &= \mathrm{rank}(\sin 2\Theta) \\ &= \mathrm{rank}(M_2) \\ &= \mathrm{rank}(P_2) \\ &\le \min(r, m-r) \equiv s \ . \end{aligned}$$

If any of the s singular values of P_2 is zero then $\rho_D < s$ and the angles $\theta_1 = \cdots = \theta_{r-\rho_D} = 0$. In this case the analog to (14), namely

$$H_- = I - G_- G_-^t \tag{16}$$

where

$$G_- = \sqrt{2}\begin{pmatrix} Q_1\sin\Theta \\ -Q_2\cos\Theta \end{pmatrix} , \tag{17}$$

fails in the sense that $H(D) \ne H_-$. For it is clear that $\mathrm{rank}(G_-) = s$, so that H_- reverses an s-dimensional subspace; but $H(D)$ reverses only $R(D)$, which is just ρ_D-dimensional. Since, by assumption, $\rho_D < s$, the two block reflectors must differ.

By Theorem 3, however, $H(D)$ is not unique. We may therefore ask whether H_- satisfies $H_-P = \overline{Q_1}$ despite the fact that it is not $H(D)$. According to Theorem 2, it does if

$$R(D) \subseteq R(G_-) \tag{18}$$

and

$$G_-^t S = 0\,. \tag{19}$$

But (18) follows from the characterization (11) of D and the definition (17) of G_-. The orthogonality (19) follows from property (8) of Q_2.

When D is rank deficient there may be other choices as well. In fact, if $\rho_D < s-1$ then there are block reflectors that reflect P into $\overline{Q_1}$ and reverse subspaces of dimension greater than ρ_D and less than s. The two that we have exhibited are the extreme cases: $H(D)$ reverses the smallest possible subspace $[R(D)]$, while H_- reverses the largest $[R(S)^\perp]$.

2.6.1. Other choices for F. Were we to take any other orthogonal-symmetric factorization (Q_1M_1 with M_1 indefinite) of P_1, we could still construct block reflectors $H_\pm$ by (14) and (16). Now, in general, neither $H(S) = H_+$ nor $H(D) = H_-$. But nevertheless, $H_\pm P = \mp\overline{Q_1}$.

2.6.2. Other representations for H. When $m = 2r$ we may write

$$H_\pm = \mp(Q_1 \oplus Q_2)\begin{bmatrix}\cos 2\Theta & \sin 2\Theta\\ \sin 2\Theta & -\cos 2\Theta\end{bmatrix}(Q_1 \oplus Q_2)^t\,,$$

in exact analogy to the elementary case. In general, $m \neq 2r$ and we have that

$$H_\pm = \begin{pmatrix}0 & 0\\ 0 & I - Q_2Q_2^t\end{pmatrix} \mp (Q_1 \oplus Q_2)\begin{bmatrix}\cos 2\Theta & \sin 2\Theta\\ \sin 2\Theta & -\cos 2\Theta\end{bmatrix}(Q_1 \oplus Q_2)^t\,.$$

3. Applications and computation.

3.1. Applications.

1. *Optimal error bounds.* Let the columns of U be approximate eigenvectors for some symmetric $A \in \mathbf{R}^{m\times m}$. Let $\Lambda = \operatorname{diag}(\theta_1, \cdots, \theta_n)$ be approximate eigenvalues. Let $X := AU - U\Lambda$ be a residual matrix. Next map X into its mirror image $\binom{Y}{0}$ by a suitable block reflector H. Then form the auxiliary symmetric matrix

$$T = T(V) = \begin{pmatrix}\Lambda & Y^t\\ Y & V\end{pmatrix}$$

where V is at our disposal.

By choosing suitable V and computing the eigenvalues of $T(V)$ error bounds may be obtained on the approximate values $\theta_1, \cdots, \theta_n$. In several important cases

V can be chosen so that the bounds are optimal for the given information. See [11, §§10–4 — 10–9] for more details.

The point of interest here is that the residual matrix X is likely to have lower rank than is revealed by its columns alone.

2. *Block Hessenberg form.* It is possible to reduce a matrix $B \in \mathbf{R}^{m \times m}$ to block upper Hessenberg form by explicit orthogonal similarity transformations

$$B \to C = H^t B H = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} \\ 0 & C_{32} & C_{33} & C_{34} & C_{35} \\ 0 & 0 & C_{43} & C_{44} & C_{45} \\ 0 & 0 & 0 & C_{54} & C_{55} \end{bmatrix}.$$

Here H represents a product of three block reflectors, $H = H_1 H_2 H_3$. The first step is typical. We seek H_1 so that

$$H_1 \begin{bmatrix} B_{21} \\ B_{31} \\ B_{41} \\ B_{51} \end{bmatrix} = \begin{bmatrix} C_{21} \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

In tnese circumstances we expect full rank to be maintained. It may not pay to try and represent $H_1 = I_m - G_1 G_1^t$ where $G_1 \in \mathbf{R}^{m \times r}$ since usually $r = n$.

Block QR factorizations can be computed in a similar manner, by applying a sequence of block reflectors to a matrix [2,4].

3.2. Stable computation of the block reflector. Recall that $E \in \mathbf{R}^{m \times n}$ is given and we seek a block reflector $H = H(Z)$ such that $HE = \overline{F} = \binom{F}{0}$ for some $n \times n$ matrix F. In this section we shall describe four elegant and stable constructions for mirror images F of E and of matrices $G \in \mathbf{R}^{m \times r}$ such that $G^t G = 2I_r$ and the block reflector $H = I - GG^t$ maps between $R(E)$ and $R\left(\begin{bmatrix} I \\ 0 \end{bmatrix}\right)$. One of these, Algorithm 2, appears in a slightly different form in [4].

As in §2.6, we suppose we have a matrix $P \in \mathbf{R}^{m \times r}$ such that $R(E) \subset R(P)$ and P has orthonormal columns. Thus $P^t P = I_r$, and $E = PT$ for some $T \in \mathbf{R}^{r \times n}$. We can easily find T since

$$T = P^t E.$$

Let $P = \begin{bmatrix} P_1 \\ P_2 \end{bmatrix}$ with P_1 square. Let $P_1 = Q_1 M_1$ be a polar decomposition of P_1. The orthogonal polar factor Q_1 is a mirror image of P. With this choice,

$$S = \begin{bmatrix} Q_1 + P_1 \\ P_2 \end{bmatrix}. \tag{20}$$

Then as we have seen, $H = H(S)$ satisfies $HP = \begin{bmatrix} -Q_1 \\ 0 \end{bmatrix}$, which is our objective.

It remains only to find a convenient representation for H. The one given by (14)-(15) is a possibility. We shall compute the necessary matrices $\cos\Theta$ and $\sin\Theta$ using (9). In the computation of $\sin\Theta$, however, it is possible that cancellation of nearly equal elements on the diagonal can spoil the formation of $I - M_1$. Following [11, p. 91] in the one-dimensional case, we may use the relation

$$\begin{aligned} I - M_1 &= (I + M_1)^{-1}(I - M_1^2) \\ &= (I + M_1)^{-1}(I - P_1^t P_1) \\ &= (I + M_1)^{-1}(P_2^t P_2) \end{aligned}$$

to construct $I - M_1$ without any matrix subtraction.

This leads to the following algorithm. Recall that $M_1 = \cos 2\Theta$ and $M_2 = \sin 2\Theta$.

ALGORITHM 1. *Compute $F \in \mathbf{R}^{n\times n}$ and $G_+ \in \mathbf{R}^{m\times r}$, $r \leq n$, such that $H_+E = \overline{F}$, where $H_+ \equiv I - G_+G_+^t$.*

1. Find $P \in \mathbf{R}^{m\times r}$ and $T \in \mathbf{R}^{r\times n}$ such that $R(E) \subseteq R(P)$, $P^tP = I$, and $PT = E$;
2. $[Q_1, M_1] :=$ polar(P_1) and $[Q_2, M_2] :=$ polar(P_2), where $P = \binom{P_1}{P_2}$;
3. $F := \begin{pmatrix} -Q_1T \\ 0_{n-r\times n} \end{pmatrix}$;
4. $\cos\Theta := (I + M_1)^{1/2}$ and $\sin\Theta := \left((I + M_1)^{-1}P_2^tP_2\right)^{1/2}$;
5. $G_+ := \begin{bmatrix} Q_1\cos\Theta \\ Q_2\sin\Theta \end{bmatrix}$.

In Step 1, the required orthonormal matrix P may be obtained using a QR-factorization of E, with column pivoting if we wish r to be minimal and $R(E) = R(P)$.

There are no additional difficulties in computing G_- and H_- according to (16)-(17). Only Step 5 of Algorithm 1 needs to be replaced, by

5a. $G_- := \begin{bmatrix} Q_1\sin\Theta \\ -Q_2\cos\Theta \end{bmatrix}$.

We give the resulting algorithm the name "Algorithm 1a".

The two polar decompostions and two square roots add to the cost of Algorithm 1. It may well be that the cost of applying H to some large matrix so dominates the cost of contructing it that this is insignificant. We shall try, nevertheless, to reduce this initial cost by seeking alternatives to the representation given by (14)-(15). We therefore seek a new representation of H as $I - G'_+(G'_+)^t$ where $G'_+ \in \mathbf{R}^{m\times r}$. By (20), or equally well by (9) and (13),

$$\begin{aligned} \tfrac{1}{2}S^tS &= \tfrac{1}{2}\left[Q_1^tQ_1 + P^tP + 2Q_1^tP_1\right] \\ &= I + M_1\,. \end{aligned} \tag{21}$$

Now let R be the upper triangular Cholesky factor of $I + M_1$. Since the eigenvalues of $I + M_1$ are all in $[1, 2]$, both R and $I + M_1$ are extremely well conditioned. Define

$$G'_+ = \begin{bmatrix} Q_1 R^t \\ P_2 R^{-1} \end{bmatrix} .$$

Then

$$\begin{aligned} G'_+ &= \begin{bmatrix} Q_1(I + M_1) \\ P_2 \end{bmatrix} R^{-1} \\ &= \begin{bmatrix} Q_1 + P_1 \\ P_2 \end{bmatrix} R^{-1} \\ &= S R^{-1} . \end{aligned} \tag{22}$$

Thus, by (21) and (22),

$$\begin{aligned} H(S) &= I - S(\tfrac{1}{2} S^t S)^{-1} S^t \\ &= I - S R^{-1} R^{-t} S^t \\ &= I - G'_+ (G'_+)^t . \end{aligned}$$

Thus we have a second algorithm.

ALGORITHM 2. *Compute $F \in \mathbf{R}^{n \times n}$ and $G'_+ \in \mathbf{R}^{m \times r}$, $r \leq n$, such that $HE = \overline{F}$, where $H \equiv I - G'_+(G'_+)^t$.*

1. Find $P \in \mathbf{R}^{m \times r}$ and $T \in \mathbf{R}^{r \times n}$ such that $R(E) \subseteq R(P), P^t P = I$, and $PT = E$;
2. $[Q_1, M_1] :=$ polar(P_1) where $P = \binom{P_1}{P_2}$;
3. $F := \begin{pmatrix} -Q_1 T \\ 0_{n-r \times n} \end{pmatrix}$;
4. $R :=$ cholesky$(I + M_1)$;
5. $G'_+ := \begin{bmatrix} Q_1 R^t \\ P_2 R^{-1} \end{bmatrix}$.

Thus we may represent H_+ without having to construct $\sin \Theta$ or $\cos \Theta$. It is worthwhile asking whether we can do the same for H_-. We seek G'_- such that $H_- = I - G'_-(G'_-)^t$. We may attempt to repeat the derivation above, substituting $-Q_1$ for Q_1. But there is a cause for concern. The Cholesky factor of $I - M_1$ and its inverse may not exist or, worse, may be ill conditioned.

Instead we proceed as follows. Define $P_- \equiv \frac{1}{2} G_- G_-^t$ where G_- is given by (17).

Then $H_- = I - 2P_-$. Furthermore, using (9),

$$\begin{aligned}
2P_- &= 2\begin{pmatrix} Q_1 \sin\Theta \\ -Q_2\cos\Theta \end{pmatrix}\begin{pmatrix} Q_1 \sin\Theta \\ -Q_2\cos\Theta \end{pmatrix}^t \\
&= \begin{pmatrix} Q_1 \sin 2\Theta \\ -Q_2(2\cos^2\Theta) \end{pmatrix}(2\cos^2\Theta)^{-1}\begin{pmatrix} Q_1 \sin 2\Theta \\ -Q_2(2\cos^2\Theta) \end{pmatrix}^t \\
&= \begin{pmatrix} Q_1 M_2 R^{-1} \\ -Q_2 R^t \end{pmatrix}\begin{pmatrix} Q_1 M_2 R^{-1} \\ -Q_2 R^t \end{pmatrix}^t \\
&\equiv G'_-(G'_-)^t .
\end{aligned}$$

To summarize, we have

ALGORITHM 3. *Compute $F \in \mathbf{R}^{n\times n}$ and $G'_- \in \mathbf{R}^{m\times r}$, $r \le n$, such that $HE = \overline{F}$, where $H \equiv I - G'_-(G'_-)^t$.*

1. Find $P \in \mathbf{R}^{m\times r}$ and $T \in \mathbf{R}^{r\times n}$ such that $R(E) \subseteq R(P)$, $P^tP = I$, and $PT = E$;
2. $[Q_1, M_1] :=$ polar(P_1) and $[Q_2, M_2] :=$ polar(P_2) where $P = \binom{P_1}{P_2}$;
3. $F := \begin{pmatrix} -Q_1 T \\ 0_{n-r\times n} \end{pmatrix}$;
4. $R :=$ cholesky$(I + M_1)$;
5. $G'_- := \begin{bmatrix} Q_1 M_2 R^{-1} \\ -Q_2 R^t \end{bmatrix}$.

Therefore we may again stably construct a representation of H_- without resort to $\sin\Theta$ and $\cos\Theta$. But in this case we must compute a polar decomposition (7) of P_2.

Thus, the essential difference between the constructions of $G_\pm$ and $G'_\pm$ is that for $G_\pm$ one uses two matrix square roots, to compute $\cos\Theta = \frac{1}{\sqrt{2}}(I + M_1)^{1/2}$ and $\sin\Theta = \frac{1}{\sqrt{2}}\left[(I + M_1)^{-1}(I - M_1^2)\right]^{1/2}$; while for $G'_\pm$ one must use a Cholesky factorization of $I + M_1$. Furthermore, one may construct G_+ without ever computing the factors Q_2 and M_2 of P_2, which is a distinct advantage.

Still other representations for $H_\pm$ are possible. For example,

1. Compute $P_1 = Q_1 M_1$ and $V = (I + M_1)^{-1}$;
2. $H_+ = \begin{pmatrix} -P_1 Q_1^t & -Q_1 P_2^t \\ -P_2 Q_1^t & I - P_2 V P_2^t \end{pmatrix}$.

3.2.1. Efficiency. Algorithms that are couched in terms of modules such as the Basic Linear Algebrta Subprograms [9], matrix-vector products, and matrix-matrix products tend to perform well on modern vector and parallel computers [5]. In fact, very high speed systolic array devices can be used to implement these operations. One advantage of block reflectors is that they can be computed using matrix multiplication for most of the work, and they can be applied using matrix multiplication for all of the work. Bischof and Van Loan [1] point out that algorithms "rich in matrix multiplication" are attractive for these reasons. Matrix multiply $(n \times n)$ also has the extremely important property that there is substantial reuse of data - $O(n^2)$ data and $O(n^3)$ arithmetic. It is therefore possible to support a processor whose speed is $O(n)$ times greater than the bandwidth of the memory.

In Algorithm 2 above, computation of a block reflector requires

[i] Computation of an orthonormal matrix P such that $E = PT$;

[ii] Polar decomposition of an $n \times n$ matrix;

[iii] Cholesky factorization of an $n \times n$ matrix and inversion of the Cholesky factor;

[iv] Matrix multiplication.

As applied to computation of the block reflector, the operation counts of items [i] and [iv] are $O(mn^2)$ and those of items [ii] and [iii] are $O(n^3)$. We are especially interested in the case $m \gg n$.

The computation of P (item [i]) could be done using a QR factorization (with column pivoting if we wish to make the number of columns of P as small as possible). The implementation suggested by Bischof and Van Loan, which is rich in matrix multiply, could be used. In a later paper, we shall give another algorithm for item [i] that is rich in matrix multiply.

Item [iii] is not matrix multiply, but it is very inexpensive compared to the other items.

The polar decomposition, item [ii], can also be computed with a procedure dominated by matrix multiply. We start with Higham's method for the polar decomposition of a given nonsingular matrix A. In brief, this algorithm constructs a sequence of matrices $\{B_i\}$ where

$$B_0 = A$$

and

$$B_{i+1} = \frac{1}{2}(\gamma_i B_i + \frac{1}{\gamma_i} B_i^{-T})$$

and the scalars γ_i are chosen by the algorithm to accelerate convergence. The sequence $\{B_i\}$ converges quadratically to the orthogonal polar factor. Higham has shown that 5-6 iterations are typically needed and that the computation time is somewhat less than that for the usual SVD-based method [7].

At each step, B_i^{-1} is needed; its computation dominates, only $O(n^2)$ other work is done. For the first step, the inverse can be computed in a conventional way. For all the subsequent iterations of Higham's method, we take advantage of the fact that B_{i-1}^{-1} is a good *a priori* approximation to B_i^{-1}, which gets better with increasing i due to the rapid convergence of $\{B_i\}$. In fact,

$$\|B_{i+1} - B_i\| = O(2^{-2^i}) .$$

It follows, since $B_\infty = Q$ is orthogonal and hence has condition number unity that

$$\|B_{i+1}^{-1} - B_i^{-1}\| = O(2^{-2^i}) .$$

Therefore we use Schulz's iterative method [12] as an inner iteration to compute B_i^{-1}. This matrix iteration produces a sequence $\{A_k\}$ via

$$A_{k+1} = A_k + (I - A_k B_i) A_k . \quad k = 0, 1, \ldots$$

where

$$A_0 = B_{i-1}^{-1} .$$

The sequence $\{A_k\}$ converges to B^{-1} quadratically.

Note that this method is entirely matrix multiply-add. Experiments have shown that five iterations suffice for convergence of Higham's method. The question is, how many iterations of Schulz's method are required. This depends on i. Here are typical results:

Iteration i	Number of inner iterations k
1	6
2	5
3	3
4	2
5	1

Thus, about 17 Schulz iterations, or 34 matrix multiplications, are needed for the polar factorization. Were the matrix inverses to be computed directly, five such inverses would have been necessary. Since matrix inversion requires as many floating point operations as matrix multiplication ($2n^3$), the matrix multiply oriented version of the algorithm is more efficient if matrix multiply can be done at a rate $34/5 =$ 6.8 times faster than matrix inversion.

The SVD can also be used to compute a polar factorization. Higham has shown that his algorithm is somewhat less costly, even under the usual model of computational cost.

4. Experiments. Ten very ill-conditioned 12×8 matrices E were generated by the following procedure. Random matrices U_1 and V_1 were chosen and their columns orthogonalized to produce orthogonal matrices U and V. Seven random singular values were obtained by sampling the random variable

$$\sigma := \epsilon^{1-\mu^2}$$

where $\epsilon = 2^{-52}$ was the machine precision and μ was uniformly distributed in [0, 1]; the other singular value was taken to be 1. Finally we computed

$$E = U\Sigma V^t ,$$

where $\Sigma = \mathrm{diag}(\sigma_1, \cdots, \sigma_8)$. We then computed a $12 \times r$ matrix P with orthonormal columns, and $\mathrm{rank}(E) \leq r \leq 8$. Algorithm 2 was used to find F and G'_+. All computations were performed on an IBM PC/AT using PC MATLAB, which employs IEEE-standard double precision arithmetic, with 15 decimal-digit precision.

Let

$$H = I - G'_+(G'_+)^t = \begin{bmatrix} H_1 \\ H_2 \end{bmatrix}, \quad H_1 \in \mathbf{R}^{8\times 12}.$$

In each case we computed four measures of error.

1. (nonorthogonality): $\|I_{12} - H^t H\|$;
2. (anisometry): $\|F^t F - E^t E\|$;
3. (correctness of F): $\|H_1 E - F\|$;
4. (correctness of H): $\|H_2 E\|$.

The matrix 2-norm was used. The rank of P varied from 3 to 7. The condition number of E was always at least 2.7×10^{15}. All the error measures were in the interval $[0, .7 \times 10^{-14})$.

Isomorphic experiments were performed using G'_- (computed using Algorithm 3), G_+ (computed using Algorithm 1), and G_- (computed using Algorithm 1a), with these results:

0. Errors using G'_+ were $\leq .7 \times 10^{-14}$;
1. Errors using G'_- were $\leq .7 \times 10^{-14}$;
2. Errors using G_+ were $\leq .9 \times 10^{-14}$;
3. Errors using G_- were $\leq 3.0 \times 10^{-14}$.

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13. ABSTRACT

A block reflector is an orthogonal, symmetric matrix that reverses a subspace whose dimension may be greater than one. We shall develop the properties of block reflectors and give some algorithms for computing a block reflector that introduces a block of zeros into a matrix. We consider the compact representation of block reflectors, some applications, and their use in parallel computers. (LF)

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